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Institute for Multiscale Materials Distinguished Lecture Series

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The Nanostructure of Nafion for Fuel-Cell Membranes: Small-Angle Scattering and NMR Analysis

Thursday, May 5, 2011
2:00 - 3:00 P.M.
Research Park, TA-3, Bldg. 4200, Suite 101A
Access Grid Conference Room

Abstract: We have investigated the long contentious nanometer-scale structure of hydrated Nafion, a benchmark material for proton exchange membranes in H2/O2 fuel cells. 13C and 19F NMR results highlight the significant stiffness of the perfluorinated polymer backbone. In order to obtain the maximum information about the hydrated nanoclusters in Nafion from small-angle scattering data, we have developed an algorithm, based on 3D numerical Fourier transformation, that yields the scattered intensity I(q) for any model implemented on a cubic lattice. Using this approach, we have quantitatively simulated previously published small-angle scattering data of hydrated Nafion. The characteristic ”ionomer peak” is attributed to long, parallel but otherwise randomly packed water channels surrounded by the partially hydrophilic sidebranches, forming inverted-micelle cylinders. Small-angle scattering patterns of drawn Nafion strongly support this view. The channels are stabilized by the considerable stiffness of the Nafion backbones detected by NMR. An upper limit of 100 nm to the persistence length of the water channels has been estimated from 2H NMR of 2H2O diffusing in the channels. At 20 vol% water, the water channels have diameters between 1.8 and 3.5 nm, with a 2.4-nm average. The changes in small-angle scattering and in the surface-to-volume ratio with hydration level have also been analyzed. Nafion crystallites (~10 vol%), which form physical crosslinks crucial for the mechanical properties of Nafion films, are elongated and parallel to the water channels, with cross sections of ~(5 nm)2. Simulations for a dozen other models of Nafion, including Gierke’s cluster and the polymer-bundle model, do not match the scattering data. The water-channel model is the first without constrictions of ~1.2 nm diameter; it can explain important features of hydrated Nafion, in particular the fast diffusion of water and protons through Nafion.

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Bio: Professor, received his Diploma in Physics in 1989, and a Ph.D. "summa cum laude" in 1991, from the University of Mainz, Germany, working with H. W. Spiess at the Max-Planck Institute for Polymer Research. In 1992, he was a staff scientist at the Max-Planck Institute and wrote a book on "Multidimensional Solid-State NMR and Polymers" (with H. W. Spiess). He then spent two years in the group of Alex Pines at UC Berkeley, as a postdoctoral fellow of the BASF AG and the German National Scholarship Foundation. In 1995, he joined the Department of Polymer Science & Engineering of the University of Massachusetts at Amherst, where in 1997 he was promoted to Associate Professor. He joined the faculty of ISU in 2000. In 1996, he received the Rudolf-Kaiser Prize from the German Physical Society, and a Beckman Young Investigator Award from the Arnold and Mabel Beckman Foundation. In 2000, he was awarded an Alfred P. Sloan Research Fellowship, in 2001, the John H. Dillon Medal of the Polymer Division of the American Physical Society.

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